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New ExoMol line lists for PO, PS, SiH, NS and SH.

Maire N. Gorman[1, 2], Sergey N. Yurchenko[1], Jonathan Tennyson[1], Wesley Bond[1], Christian Hill[1], Pawel Jagoda[1], Lorenzo Lodi[1], William Nunn[1], Laura McKemmish[1, 3], Laxmi Prajapat[1], Rohan Shah[1], Frances Sinden[1]

1. Department of Physics and Astronomy, University College London, London WC1E 6BT, UK
2. Department of Physics, Aberystwyth University, Penglais, Aberystwyth, Ceredigion, UK, SY23 3BZ
3. School of Chemistry, University of New South Wales, Sydney, Australia, NSW 2052

Introduction

In this poster we present recently published line lists for five diatomic molecules which are of astronomical interest as detailed below:

SiH
- Detected in sunspots (Pearse 1933 and Babcock 1945) and Solar disk spectrum (Schadee 1964 and Moore-Sitterly 1966, Lambert & Mallia 1970, Grevesse & Sauval 1971).
- Detected in late type stars (Davis 1940) and M- and S-type Mira variable stars (Merrill 1955).
- Of interest in M-dwarf atmospheres (Allard & Hauschildt 1995).
- Prediction that should be present in exoplanetary & brown dwarf atmospheres (Visscher et al. 2010).
- Candidate for ISM clouds (Herbst et al. 1989).

SH
- Challenging to detect due to location of key rotational transition.
- Detection in AGB stars (Yamamura et al. 2000) & Sun's atmosphere (Berdyugina & Livingston 2002).
- Tentatively detected in comets (Krishna Swamy & Wallis 1987, 1988).
- Following extensive searches, Neufeld et al. (2012) detected SH in the ISM using SOFIA.
- Predicted tooccur in brown dwarfs (Visscher et al. 2006) and hot Jupiter exoplanets (Visscher et al. 2006; Zahnle et al. 2009).

NS
- One of first ten diatomic molecules to be detected in space (Somerville 1977; Lovas et al. 1979).
- Detected in giant molecular clouds (McGonagle et al. 1992; Leurini et al. 2006; Belloche et al. 2013), cold dark clouds (McGonagle et al. 1994), comets (Irvine et al. 1999; Biver 2005), extragalactically (Marttn et al. 2003) and the NGC 253 starburst region (Meier et al. 2015).

PO

Detected in the following:
- Red Supergiant Star VY Canis Majoris (Tenenbaum et al. 2007).
- Oxygen-rich AGB star IK Tauri (De Beck et al. 2013).
- Star-forming regions (Lefloch et al. 2016; Rivilla et al. 2016).

PS
- No detection in space yet.
- A systematic attempt at its astronomical detection was performed by Ohishi et al. (1988).
- Local thermodynamic equilibrium calculations by Tsuji (1973) indicate that PS should be the major P-bearing molecule in oxygen-rich circumstellar envelopes for temperatures below 2000 K.

Fig 1. Potential energy curves of SiH used in the line list production. The $X^2\Pi$ and $A^2\Delta$ PECs have been refined, the $a^4\Sigma^-$ is *ab initio* and the $B^2\Sigma^-$ PEC is an artificial object used to improve the description of the Λ-doubling in the X-state spectra.

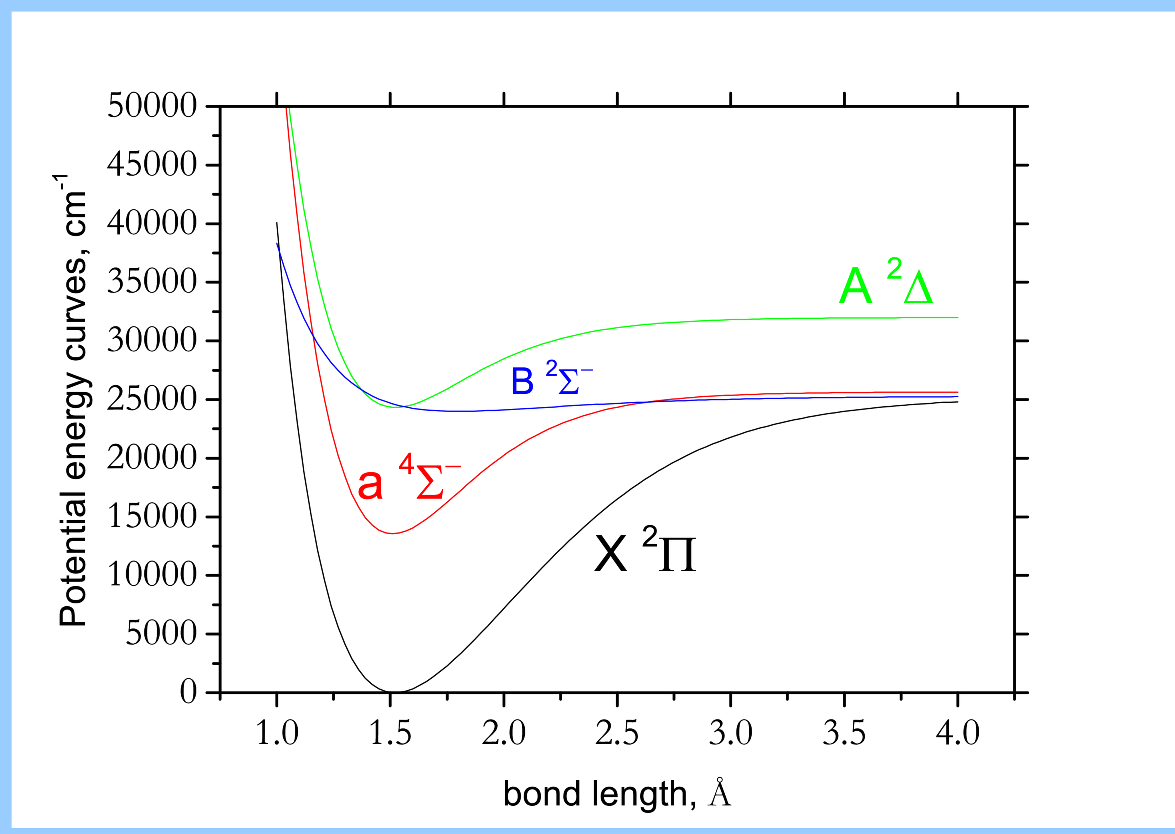


Fig 2. Comparison of simulated spectra using the new ExoMol line list for ^{32}SH with the CDMS database for the ν = 0 band.

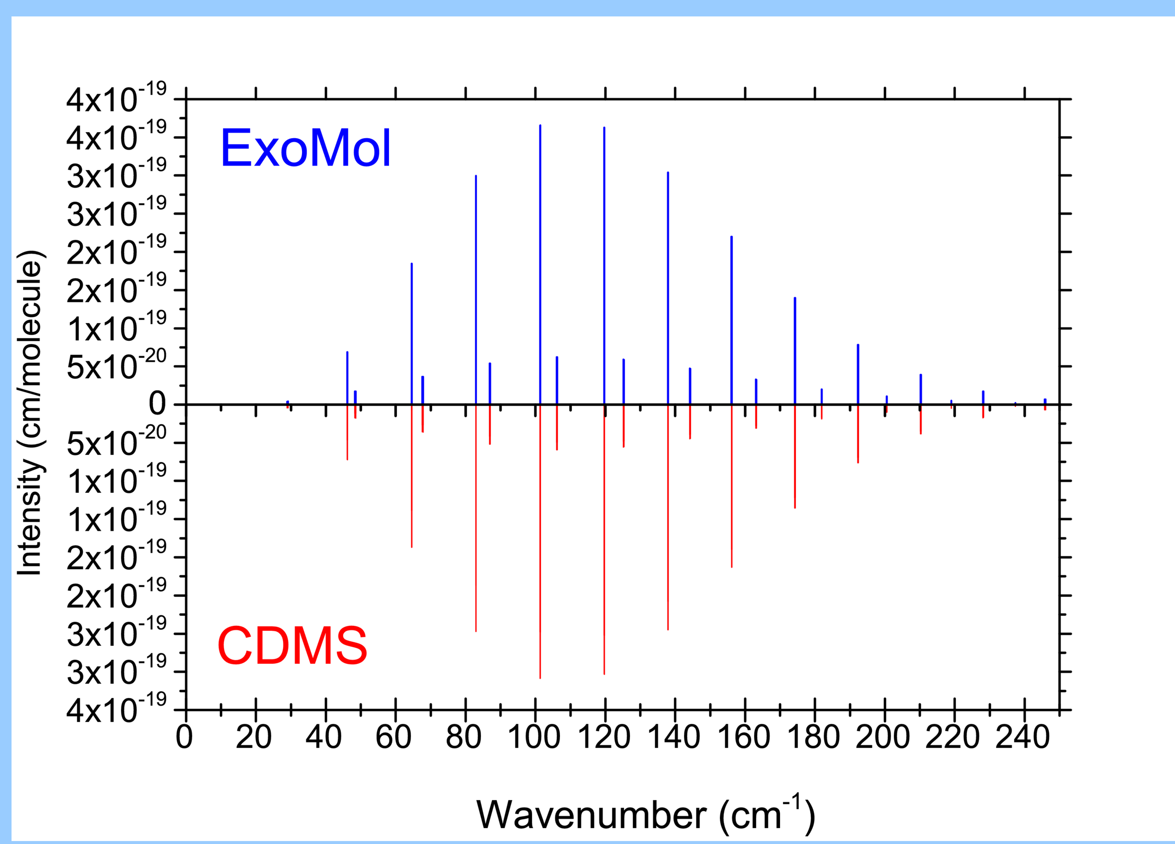


Fig 3. PO absorption spectrum at T= 300 (bottom), 1000, 2000 and 3000 (top) K, presented with cross-sections on a logarithmic scale. A Gaussian profile with HWHM=10 cm^{-1} was used.

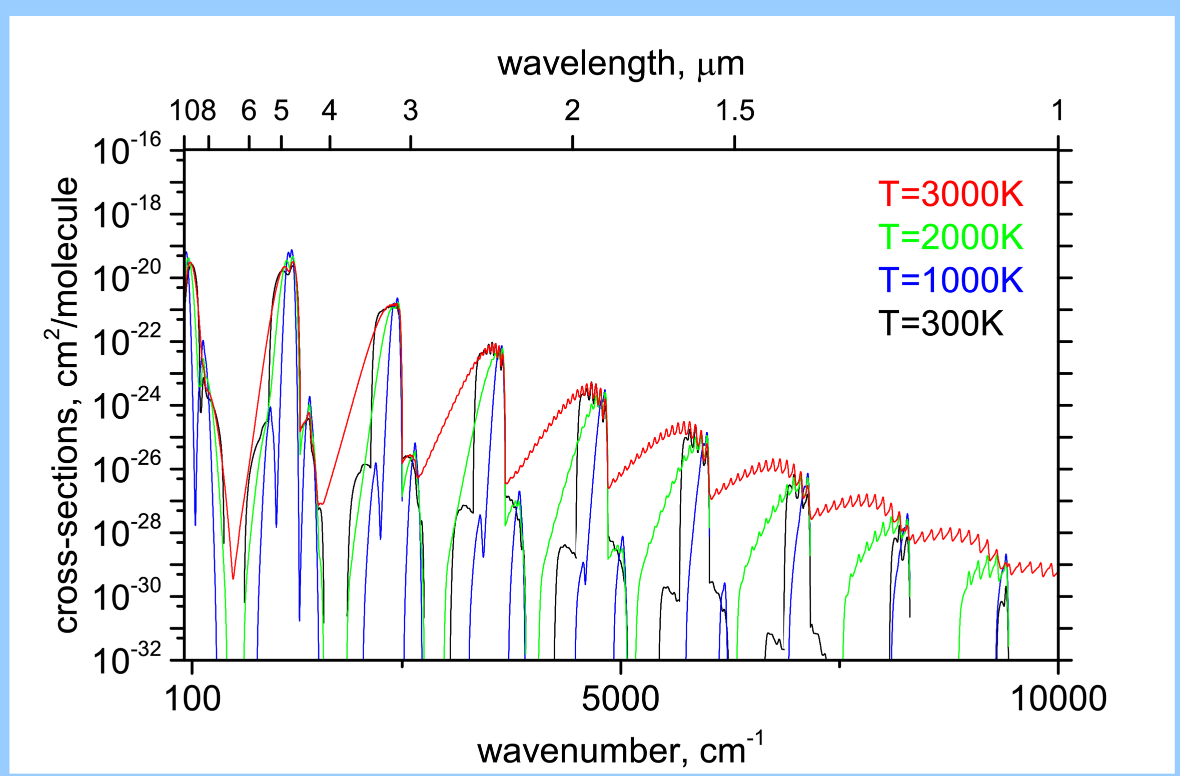


Fig 4. T = 2000 K absorption spectra of 28 SiH: X – X, a–X, and A –X bands, where the a – X band is dipole forbidden.

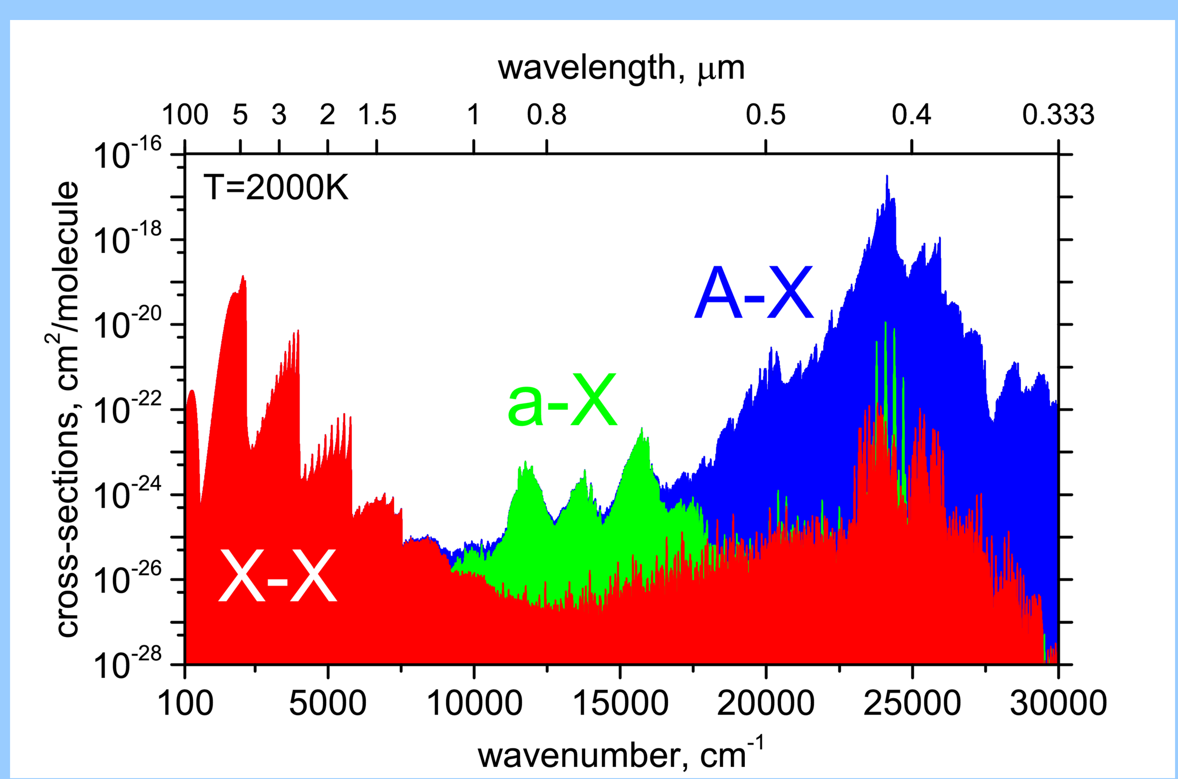


Table 1. Overview of line lists calculated. Here the number of states and transitions is quoted to the nearest 100.

Isotopologues	Jmax	Energies	Transitions
^{28}SiH, ^{29}SiH, ^{30}SiH	82.5	11 800	1 726 000
^{28}SiD	113.5	21 200	3 521 000
^{32}SH, ^{33}SH, ^{34}SH, ^{36}SH	60.5	2 300	81 300
^{32}SD	84.5	4 500	219 500
^{14}N^{32}S, ^{14}N^{33}S, ^{14}N^{34}S, ^{14}N^{36}S	235.5	31 800	3 331 000
^{15}N^{32}S	240.5	33 100	3 479 000
^{31}P^{16}O	234.5	43 100	2 096 000
^{31}P^{32}S	320.5	226 00	30 395 00

Methodology

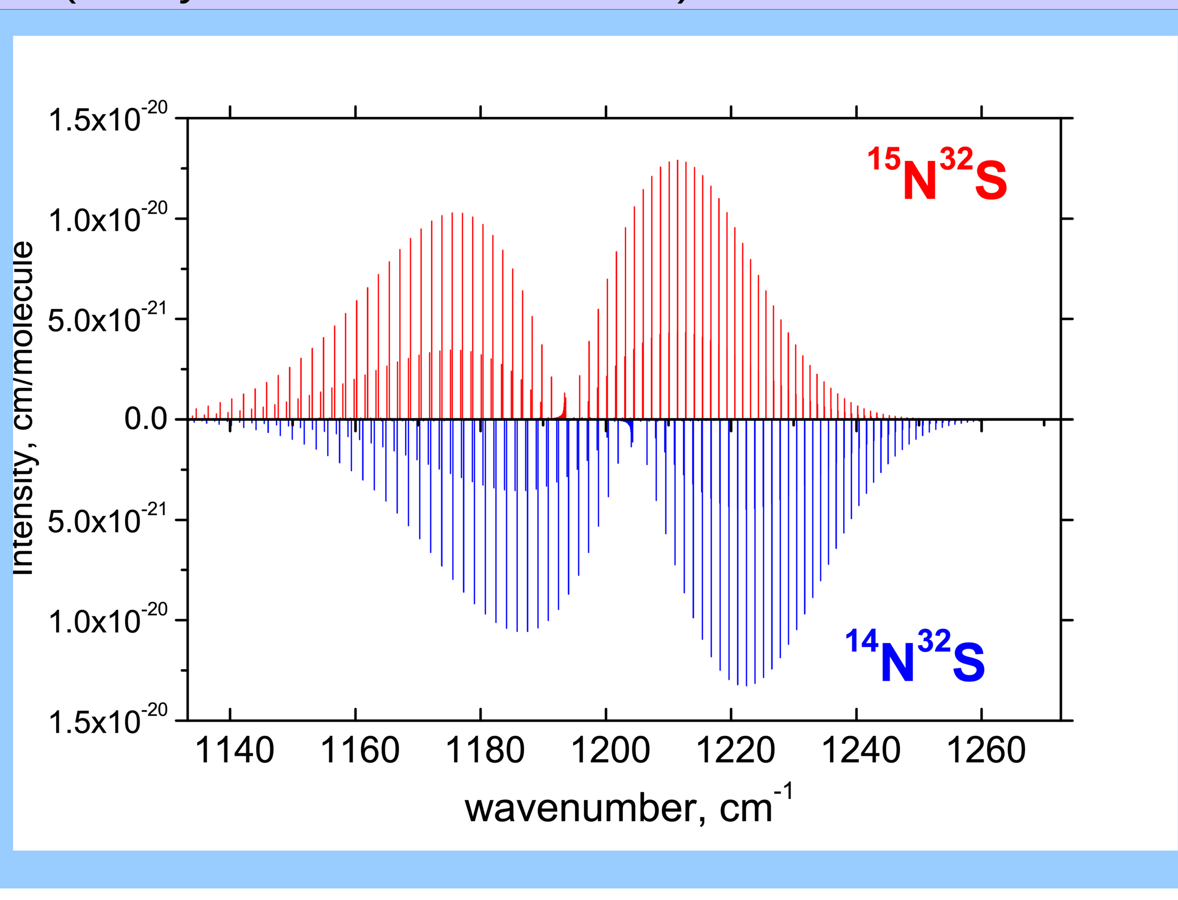
For each of the five molecules, high-level *ab initio* MRCI calculations were performed using the quantum chemistry package MOLPRO for the ground electronic state which happens to be $X^2\Pi$ for all. Additionally calculations for the $a^4\Sigma^-$, $A^2\Delta$, $B^2\Sigma^-$ states were performed for SiH, the $A^2\Sigma^+$ for SH and $a^4\Pi$, $B^2\Pi$ states for PS.

Experimental data was than compiled, analysed and then used to refine the *ab initio* Potential Energy Curves (PECs) by fitting to an Extended Morse Oscillator with an a typical accuracy of between 0.001 cm^{-1} and 0.03 cm^{-1}. In order to reduce the numerical noise when computing the line-strengths using the Duo program, we followed the recommendation by Medvedev et al. (2016) and represented these two DMCs analytically.

Using these refined curves, the coupled rovibronic Schroedinger equation was then solved to produce line lists by using the program DUO (Yurchenko et al. 2016) which has been developed within the ExoMol group specifically for diatomic molecules. The advantage of these line lists over existing experimentally compiled line lists is in terms of completeness i.e. higher vibrational and rotational coverage.

Spectra was then generated from the computed line lists using ExoCross (Tennyson & Yurchenko 2017).

Fig 5. Comparison of spectra (298 K) for the fundamental ν = 1 − 0 band of NS for ^{15}N^{32}S against ^{14}N^{32}S.



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